Ask Dr. ALOHA:

How Can You Tell Whether a Chemical is Pure?

Just a few days ago, the volunteer fire department in Little Falls, New Hampshire, installed CAMEO for the first time. Firefighter Bill Newton, the department's resident computer jockey, has already tried out all the example problems in the ALOHA manual. On a sunny October afternoon, the firefighters are called to the scene of a hazmat spill. A tank truck bound for the local airport has slid off a highway embankment, and jet fuel spilled from a tank rupture has pooled in a ditch, where it has begun to evaporate. The firefighters ask Bill whether this is a scenario they can run in ALOHA. What should Bill tell them?

There's a key question Bill should ask himself before he answers his colleagues: *Is jet fuel a pure chemical?*

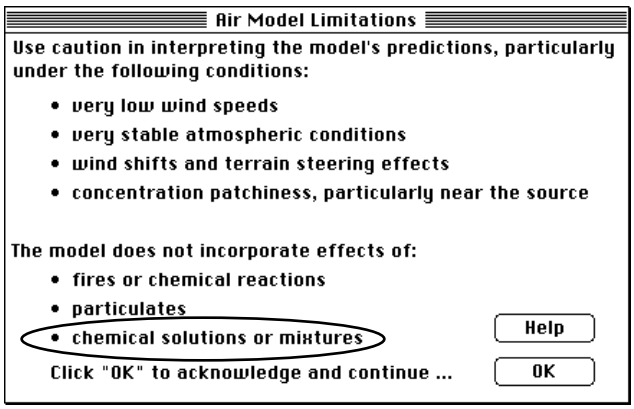
Any substance fits into one of two categories. It's either

- a **pure chemical**, composed of molecules that all have the same formula and same structure (for the purpose of this discussion, this category includes substances that are nearly pure, but may contain a few impurities), or
- a **mixture**. If it's a mixture, it's either a heterogeneous mixture, in which different parts of the substance have different properties, or it's a **solution** (solutions are uniform throughout). **Aqueous solutions**—mixtures of water with soluble chemicals—are the commonest kind of solution encountered by hazardous materials responders.

Examples of pure chemicals are chlorine and anhydrous ammonia ("anhydrous" means "without water," indicating that this substance is pure ammonia, undiluted with water). An example of an aqueous solution is aqua ammonia, which is a solution of ammonia in water. Other common aqueous solutions include acids, such as hydrochloric acid and sulfuric acid, and formaldehyde, which is a gas when it is pure, but which is usually found as a liquid solution of formaldehyde in water (which may be called either formaldehyde solution or formalin). Many solids, such as pesticides in powder or granule form, are heterogeneous mixtures.

ALOHA models only pure chemicals

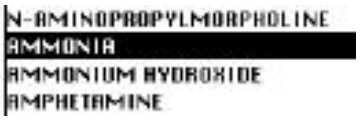
Because modeling mixtures and solutions is more computationally difficult and requires more information from users than modeling pure chemicals, ALOHA, like other air dispersion models, models only pure chemicals. Because this is such an important limitation, ALOHA alerts you about this when you first start it up (below).



Finding out whether a chemical is pure

You may already know whether the chemicals you commonly work with are pure chemicals or are mixtures or solutions. But how can you find out whether an unfamiliar substance is a pure chemical? Although it's not always easy to find this out, there are some clues to look for.

First, if a substance is included in ALOHA's library, it's a pure chemical—with some exceptions, described below. ALOHA's library contains about one-quarter of the substances included in the full CAMEO chemical database (Codebreaker and RIDS). These are all the CAMEO chemicals that are thought to be potential air hazards and that are typically (though not necessarily always) stored, transported, and used as pure chemicals. Hence, you can obtain an important clue about a substance's purity just by starting ALOHA and searching for the name of the substance in the alphabetical chemical list (to do this, from ALOHA's **SetUp** menu, choose **Chemical**). If a substance is included in the list, it's in the library and is probably a pure chemical.



However, you can't be completely certain that a chemical is pure just because it's in ALOHA's library. That's because, although all substances in ALOHA's library are commonly found in pure form, some, such as ammonia and nitric acid, also are often found in aqueous solution (mixed with water). If a chemical is mixed with water or any other substance, it is in a solution or mixture, not a pure chemical.

> **Note:** Because the information in ALOHA's library describes the pure form of each chemical, it's important not to use this information if you're instead working with a solution or mixture containing that chemical, since in such a case you're really working with a different substance. For example, if you're working with aqua ammonia, don't model it by choosing ammonia from ALOHA's library—ALOHA will model this substance as though it was anhydrous ammonia (the

pure form of ammonia), not aqua ammonia, and hence will make wrong predictions.

If you're working with a chemical that's in ALOHA's library, look for more clues to find out whether you've encountered the pure form of that chemical. One clue is a percent value in the name of the substance, which you might see on a container label. For example, "40% nitric acid" is a solution of 40 percent (by weight) nitric acid and 60 percent water. Similarly, the word "dilute" or "solution" in a substance's name indicates that the substance has been mixed with water or another solvent, and so is in a solution, not in its pure form.

Using MSDSs to check chemical purity

If you can't be sure about the purity of a chemical by checking whether it's in the ALOHA library and using other information you have on hand, such as a container label, look for an MSDS (Material Safety Data Sheet) for the chemical. An MSDS can serve as a good source of additional clues. If possible, since different formulations of some substances exist, obtain an MSDS for the substance from the manufacturer who produced it. If this isn't possible and you have access to the Internet, you can search for publicly available MSDSs for thousands of chemicals at an online repository at NOAA's Northwest Fisheries Science Center (http://research.nwfsc.noaa.gov/msds.html). This site also includes links to many other online MSDS repositories.

Once you have obtained an MSDS for a substance of concern, here are some clues to check for:

1. A list of ingredients indicates a mixture. If you see a list of ingredients on the MSDS, the substance must be a mixture of these ingredients, not a pure chemical. For example, a typical MSDS for gasoline shows the percentages of hazardous components such as cyclohexane, benzene, and toluene in a particular formulation (as in the example below).

```
==========================================================
                  Ingredients/Identity Information
==========================================================
Proprietary: NO
Ingredient: CYCLOHEXANE (SARA III)
Ingredient Sequence Number: 01
Percent: 0.2-1.6
NIOSH (RTECS) Number: GU6300000
CAS Number: 110-82-7
OSHA PEL: 300 PPM
ACGIH TLV: 300 PPM, 9293
Other Recommended Limit: NONE RECOMMENDED
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Proprietary: NO
Ingredient: BENZENE (SARA III)
Ingredient Sequence Number: 02
Percent: 1.1-4.9
NIOSH (RTECS) Number: CY1400000
CAS Number: 71-43-2
OSHA PEL: 1PPM/5STEL;1910.1028
ACGIH TLV: 10 PPM; A2; 9293
Other Recommended Limit: NONE RECOMMENDED
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Proprietary: NO
Ingredient: TOLUENE (SARA III)
Ingredient Sequence Number: 03
Percent: 7.4- 11
NIOSH (RTECS) Number: XS5250000
CAS Number: 108-88-3
OSHA PEL: 200 PPM/150 STEL
ACGIH TLV: 50 PPM; 9293
Other Recommended Limit: NONE RECOMMENDED
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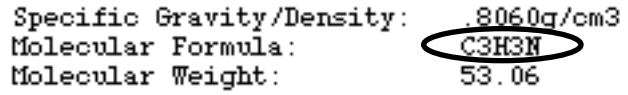
2. A single chemical formula *may* indicate a pure chemical. Some MSDSs display the chemical formula for a substance, as in the section of an MSDS for acrylonitrile, below.



When a single chemical formula is displayed, the substance is likely to be a pure chemical, unless possibly it's in aqueous solution. To check this, look for the percent concentration (if it's 100 percent, the chemical is pure), or for "solution" in the name or synonym or "dilute" in the description (either of which indicate that the substance is in solution).

You may not be able to find all the clues you need to definitely identify a substance as a pure chemical or a mixture. In such a case, it's time to turn to an expert, perhaps someone with extensive chemistry training in your organization, or a member of the chemistry department at a local college or university.

What about the spilled jet fuel?

Bill and his firefighting colleagues are still wondering about the purity of the jet fuel. Jet fuel is not in ALOHA's library, so let's take a look at an MSDS for the spilled jet fuel, which was manufactured by Northeastern Fuels. On this

MSDS, no chemical formula is shown. However, there is a list of ingredients in the jet fuel (shown below).

```
============================================================
                    Ingredients/Identity Information
============================================================
Proprietary: NO
Ingredient: ALIPHATIC PETROLEUM DISTILLATE (KEROSENE)
Ingredient Sequence Number: 01
Percent: >95
NIOSH (RTECS) Number: OA5500000
CAS Number: 8008-20-6
OSHA PEL: NOT ESTABLISHED
ACGIH TLV: NOT ESTABLISHED
Other Recommended Limit: NONE RECOMMENDED
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Proprietary: NO
Ingredient: 1,2,4-TRIMETHYLBENZENE (SARA III)
Ingredient Sequence Number: 02
Percent: 1.1
NIOSH (RTECS) Number: DC3325000
CAS Number: 95-63-6
OSHA PEL: 25 PPM
ACGIH TLV: 25 PPM; 9394
Other Recommended Limit: NONE RECOMMENDED
```

This jet fuel formulation contains more than 95 percent kerosene. Is kerosene a pure chemical? Below is part of an MSDS for deodorized kerosene. In place of a chemical formula, there's "MIXTURE OF PETROLEUM HYDROCARBONS" (below). This label indicates that kerosene is a mixture, not a pure chemical. Petroleum fuels, including kerosene and gasoline as well as jet fuel, are complex mixtures of organic chemicals called hydrocarbons. None of these fuels can be modeled in ALOHA.

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------------------------------------------------------
MSDS for   KEROSENE, (DEODORIZED)
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   1 - PRODUCT IDENTIFICATION
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PRODUCT NAME:     KEROSENE, (DEODORIZED)
FORMULA:          MIXTURE OF PETROLEUM HYDROCARBONS
FORMULA WT:             .00
CAS NO.:          08008-20-6
NIOSH/RTECS NO.:  OA5500000
COMMON SYNONYMS:  KEROSINE
PRODUCT CODES:    P339
  EFFECTIVE: 10/03/86
  REVISION #02
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The Little Falls firefighters can be sure from this information that jet fuel is a mixture of substances, not a pure chemical. Now they know that they must avoid using ALOHA to model this release. Instead, they can turn to CAMEO's RIDS module (search for "jet fuels" to view this information) and the MSDS for jet fuel to obtain response recommendations for this spill.

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